

Synthesis of polystyrene

Evaluation of protocols including a preliminary step of preparation of reagents

Protocol A^{1,2}

The greenness assessment made for protocol A did not include the preparation of reagents. If this step is considered to the greenness, the final evaluation corresponds to Figure 1. Table 1 presents the hazards and scores associated with the substances involved and Table 2 presents the scores used to construct the green stars.

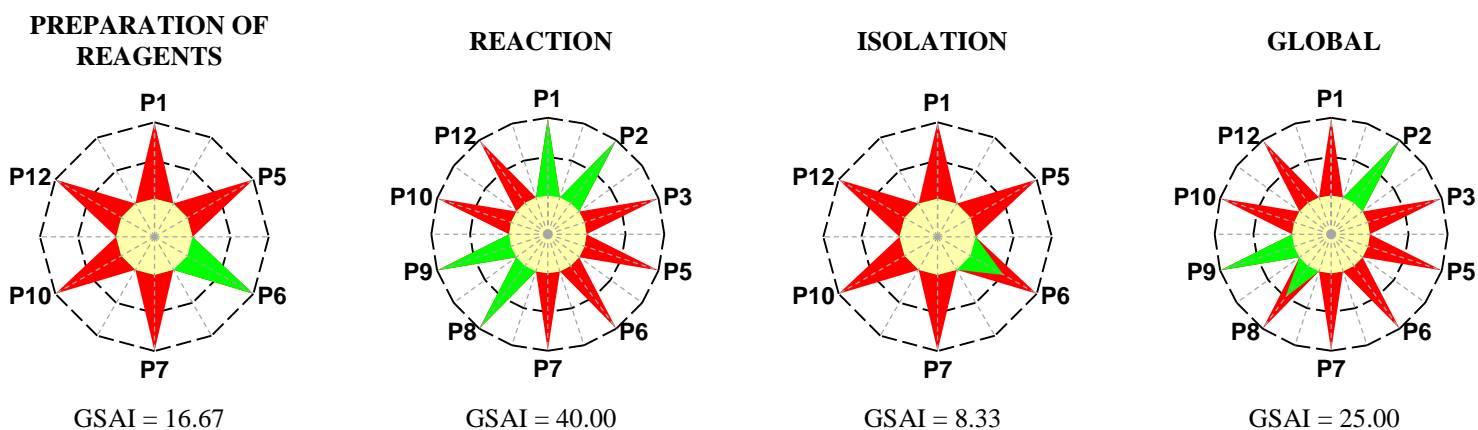


Figure 1. Greenness assessment (GS) for the synthesis of polystyrene, protocol A

Protocol C³

The greenness assessment made for protocol C did not include the preparation of reagents. If this step is considered to the greenness, the final evaluation corresponds to Figure 2. Table 3 presents the hazards and scores associated with the substances involved and Table 4 presents the scores used to construct the green stars.

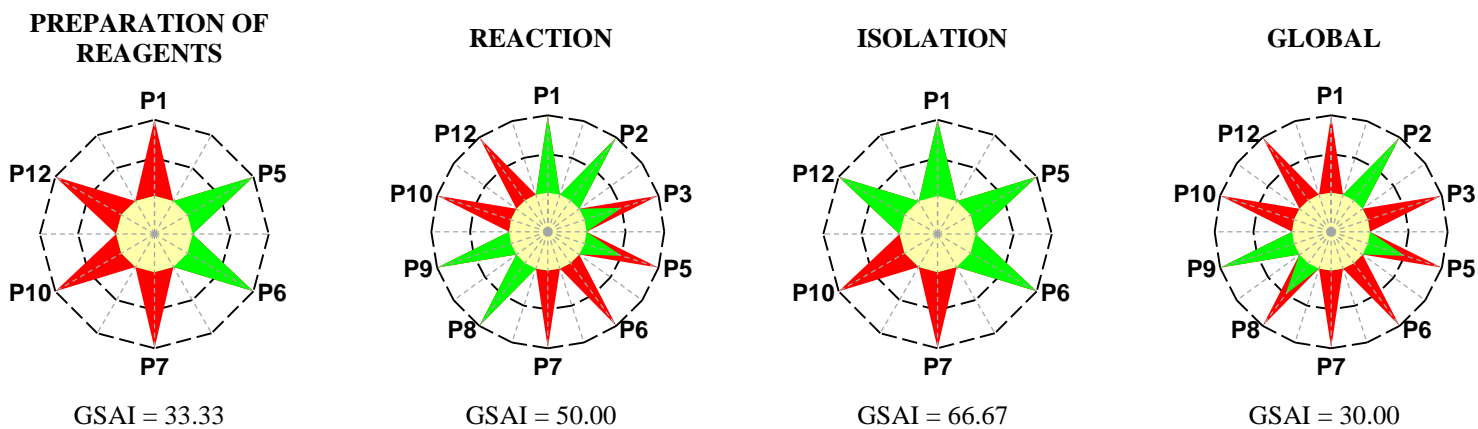


Figure 2. Greenness assessment (GS) for the synthesis of polystyrene, protocol C

Table 1. Hazards for the synthesis of polystyrene, protocol A^α

Substances involved	Step			Hazard code	Score: hazards to...		
	Prep	R	I		HH	E	P
Stoichiometric reagents							
Styrene (CAS 100-42-5)	✓	✓		H226, H315, H319, H332	2	1	2
Auxiliary substances							
Solvents							
Methanol (CAS 67-56-1)		✓	✓	H225, H301, H311, H331, H370	3	1	3
Sodium hydroxide (10% solution)	✓			H314	3	1	1
Toluene (CAS 108-88-3)		✓		H225, H304, H315, H336, H361d, H373	3	1	3
Water ^{a,b}	✓			-	1	1	1
Other auxiliary substances							
Anhydrous calcium chloride (CAS 10043-52-4)	✓			H319	2	1	1
Benzoyl peroxide (CAS 94-36-0)		✓		H241, H317, H319	2	1	3
Product							
Polystyrene (9003-53-6)		✓	✓	-	1	1	1
Waste							
4- <i>tert</i> -butylcatechol	✓			H226, H302, H311, H314, H317, H332, H370, H411	3	3	2
Calcium chloride	✓			H319	2	1	1
Methanol			✓	H225, H301, H311, H331, H370	3	1	3
Sodium hydroxide (dilute solution)	✓			-	1	1	1
Toluene	✓		✓	H225, H304, H315, H336, H361d, H373	3	1	3
Water ^{a,b}				-	1	1	1

^α Prep – Preparation of reagents; R – Reaction; I – Isolation; HH – Human Health; E – Environment; P – Physical

^a Renewable; ^b Degradable to innocuous products

Table 2. Scores used to construct the green star for the synthesis of polystyrene, protocol A ^α

Green Chemistry Principle	Preparation of reagents		Reaction		Isolation		Global	
	s	Explanation	s	Explanation	s	Explanation	s	Explanation
P1 Prevention	1	4- <i>tert</i> -butylcatechol, H311, H314, H370, H411	3	Without waste	1	Toluene, H304, H361d, H373, and methanol, H301, H311, H331, H370	1	4- <i>tert</i> -butylcatechol, H311, H314, H370, H411, toluene, H304, H361d, H373, and methanol, H301, H311, H331, H370
P2 Atom Economy		NA	3	Stoichiometric proportions of reagents, without formation of by-products		NA	3	Stoichiometric proportions of reagents, without formation of by-products
P3 Less hazardous chemical synthesis		NA	1	Toluene, H304, H361d, H373, and methanol, H301, H311, H331, H370		NA	1	4- <i>tert</i> -butylcatechol, H311, H314, H370, H411, sodium hydroxide, H314, toluene, H304, H361d, H373, and methanol, H301, H311, H331, H370
P5 Safer solvents and auxiliary substances	1	Sodium hydroxide, H314	1	Toluene, H304, H361d, H373, and methanol, H301, H311, H331, H370	1	Methanol, H301, H311, H331, H370	1	Sodium hydroxide, H314, toluene, H304, H361d, H373, and methanol, H301, H311, H331, H370
P6 Increase energy efficiency	3	Room temperature	1	T > 100 °C	2	0 °C ≤ T ≤ 100 °C	1	T > 100 °C
P7 Use renewable feedstocks	1	Substances not renewable	1	Substances not renewable	1	Substances not renewable	1	Substances not renewable
P8 Reduce derivatives		NA	3	One stage		NA	2	Two stages
P9 Catalysts		NA	3	Without catalysts		NA	3	Without catalysts
P10 Design for degradation	1	Substances not degradable	1	Substances not degradable	1	Substances not degradable	1	Substances not degradable
P12 Safer chemistry for accident prevention	1	4- <i>tert</i> -butylcatechol, H311, H314, H370, and sodium hydroxide, H314	1	Benzoyl peroxide, H241, toluene, H225, H304, H361d, H373, and methanol, H225, H301, H311, H331, H370	1	Toluene, H225, H304, H361d, H373, and methanol, H225, H301, H311, H331, H370	1	4- <i>tert</i> -butylcatechol, H311, H314, H370, sodium hydroxide, H314, benzoyl peroxide, H241, toluene, H225, H304, H361d, H373, and methanol, H225, H301, H311, H331, H370

^αs – Score; NA – Not applicable

Table 3. Hazards for the synthesis of polystyrene, protocol C^α

Substances involved	Step			Hazard code	Score: hazards to...		
	Prep	R	I		HH	E	P
Stoichiometric reagents							
Styrene (CAS 100-42-5)	✓	✓		H226, H315, H319, H332	2	1	2
Auxiliary substances							
Alumina (CAS 1344-28-1)	✓			-	1	1	1
Benzoyl peroxide (CAS 94-36-0)		✓		H241, H317, H319	2	1	3
Product							
Polystyrene (9003-53-6)		✓	✓	-	1	1	1
Waste							
4- <i>tert</i> -butylcatechol	✓			H226, H302, H311, H314, H317, H332, H370, H411	3	3	2
Alumina	✓			-	1	1	1

^α Prep – Preparation of reagents; R – Reaction; I – Isolation; HH – Human Health; E – Environment; P – Physical

Table 4. Scores used to construct the green star for the synthesis of polystyrene, protocol C^α

Green Chemistry Principle	Preparation of reagents		Reaction		Isolation		Global	
	s	Explanation	s	Explanation	s	Explanation	s	Explanation
P1 Prevention	1	4- <i>tert</i> -butylcatechol, H311, H314, H370, H411	3	Without waste	3	Without waste	1	4- <i>tert</i> -butylcatechol, H311, H314, H370, H411
P2 Atom Economy		NA	3	Stoichiometric proportions of reagents, without formation of by-products		NA	3	Stoichiometric proportions of reagents, without formation of by-products
P3 Less hazardous chemical synthesis		NA	2	Styrene, H315, H319, H332, and benzoyl peroxide, H317, H319		NA	1	4- <i>tert</i> -butylcatechol, H311, H314, H370, H411
P5 Safer solvents and auxiliary substances	3	Alumina	2	Benzoyl peroxide, H317, H319	3	Solvents and auxiliary substances are not used	2	Benzoyl peroxide, H317, H319
P6 Increase energy efficiency	3	Room temperature	1	T > 100 °C	3	Room temperature	1	T > 100 °C
P7 Use renewable feedstocks	1	Substances not renewable	1	Substances not renewable	1	Substances not renewable	1	Substances not renewable
P8 Reduce derivatives		NA	3	One stage		NA	2	Two stages
P9 Catalysts		NA	3	Without catalysts		NA	3	Without catalysts
P10 Design for degradation	1	Substances not degradable	1	Substances not degradable	1	Substances not degradable	1	Substances not degradable
P12 Safer chemistry for accident prevention	1	4- <i>tert</i> -butylcatechol, H311, H314, H370	1	Benzoyl peroxide, H241	3	Polystyrene	1	4- <i>tert</i> -butylcatechol, H311, H314, H370, and benzoyl peroxide, H241

^αs – Score; NA – Not applicable

References

- (1) Faculdade de Ciências e Tecnologia da Universidade de Coimbra,
<https://woc.uc.pt/quimica/getFile.do?tipo=2&id=1438> (accessed February 2011).
- (2) Afonso, C.A.M.; Simão, D.P.; Ferreira, L.P.; Serra, M.E.S.; Raposo, M.M.M. *100 experiências de Química Orgânica*. IST Press: Lisboa, 2011, pp. 99-102.
- (3) Williamson, K.L.; Minard, R.D.; Masters, K.M. *Macroscale and Microscale Organic Experiments – 5th edition*. Houghton Mifflin Company: Boston, 2007, pp. 826-828.